KINTECH LABORATORY

Reduced mechanism for gasoline combustion and pollutants formation at engine conditions

Background

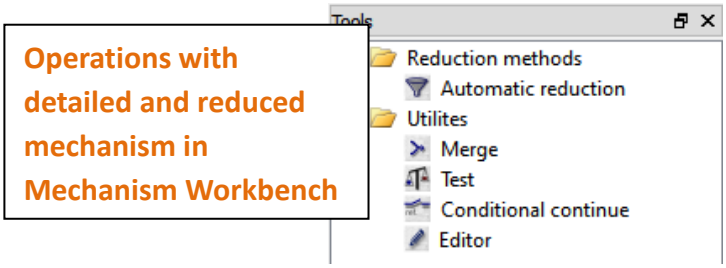
A number of processes take place in SI engines: spark ignition, turbulent flame propagation, NOx and PM formation, knock. Every process is sensitive to the combustion chemistry. In modeling studies these chemistry effects should be captured as accurate as possible. Recently detailed chemical mechanisms of PRF combustion were developed to provide this capability. The only issue is how to use these huge chemical mechanisms (>1000 species, >10000 reactions) in full-scale CFD simulations.

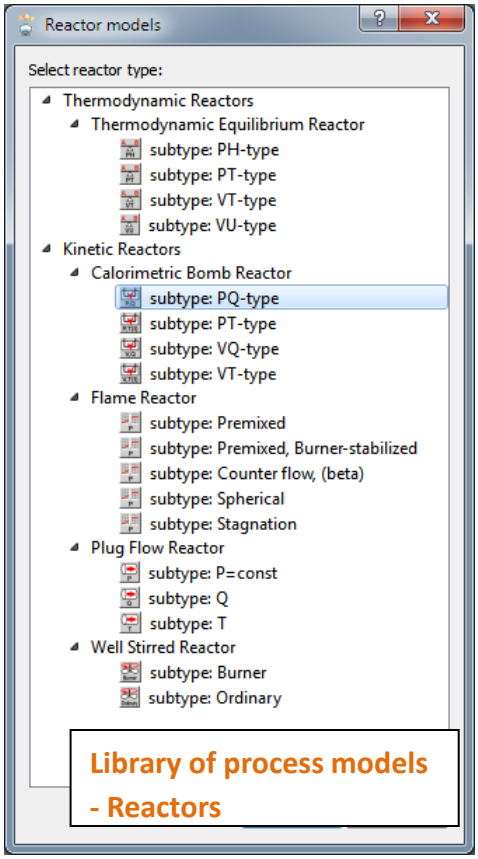
Problem statement

It is required to reduce the size of the PRF combustion mechanism [1] keeping the deviation of ignition delay time, temperature in turbulent combustion and NOx concentration, predicted with detailed and reduced mechanisms, in the range of 10%. Target conditions: stoichiometric mixture of 80% iso-octane + 20% n-hepatane, range of initial temperatures 600 – 1500K, range of pressures 20 – 40 atm.

Problem setup in Chemical Workbench

For mechanism reduction in frame of Mechanism Workbench software the Automatic Reduction tool with Kintech Lab highly efficient algorithm was used. Both redundant species and reaction were subject to removal.



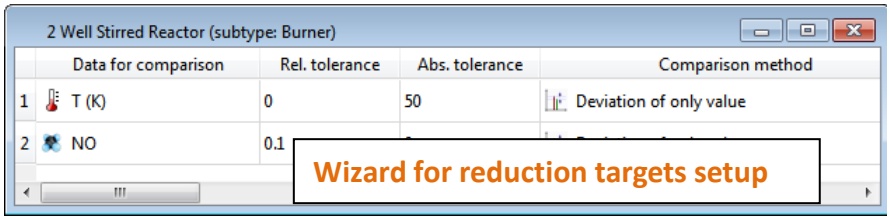


The following combustion processes were included as important for reduction

- Ignition (respective process model is Calorimetric Bomb Reactor at constant pressure and adiabatic conditions – CBR_PQ)
- Turbulent combustion and pollutants formation (respective process model is well-Stirred Reactor – WSR_Burner)

The following targets of the reduction were selected:

- For ignition
  - Ignition delay time, maximum introduced error 10%
  - Temperature (maximum introduced error 100K)
- For turbulent combustion
  - Temperature (maximum introduced error 100K)
  - NO concentration (maximum introduced error 10%)



Results

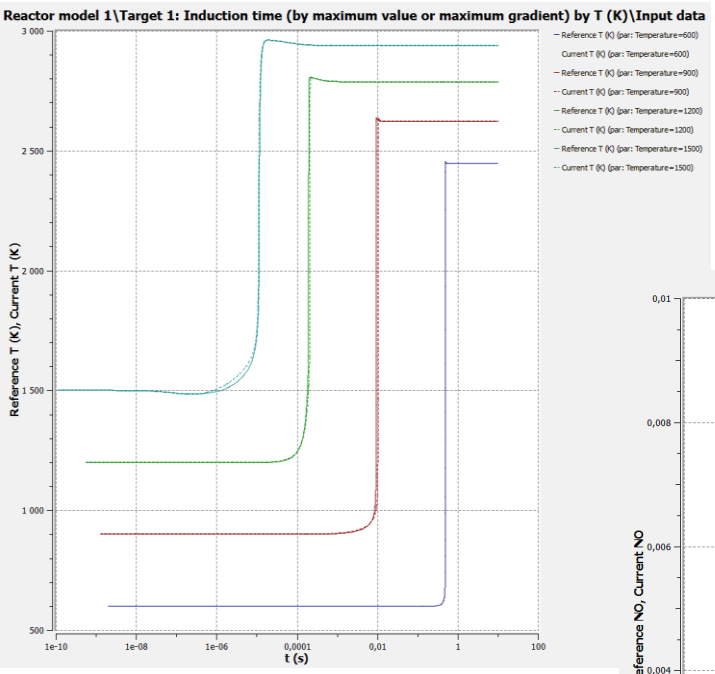
On Intel Core i7 reduction of the mechanism was done in 20 hours. It did not require any run-time monitoring and was done automatically.
The original mechanism included

- 484 species
- 19341 reactions

After reduction resulting mechanism incudes

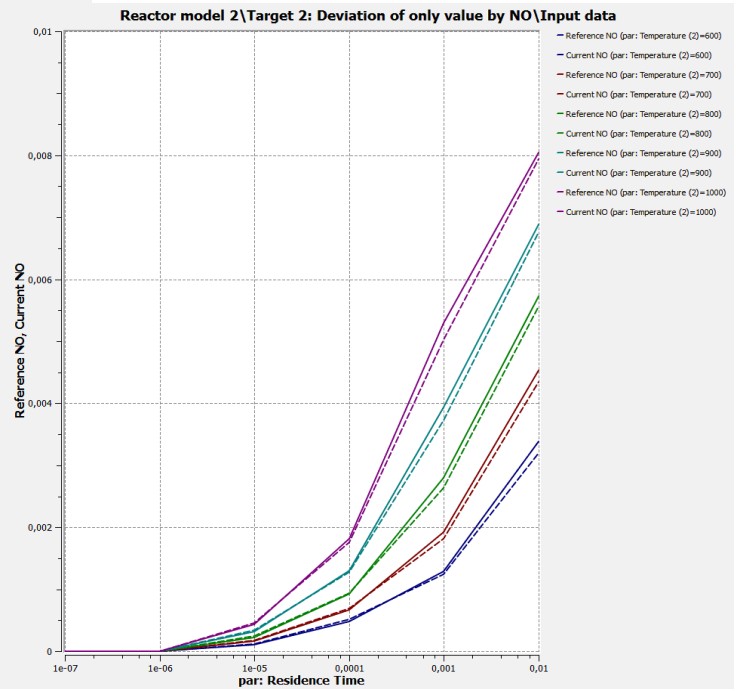
- 114 species
- 284 reactions

The reduced mechanism is able to simulate the requested combustion features (ignition delay time, temperature/heat-release profiles, NOx) with requested accuracy at given engine conditions



Reduced mechanism performance

temperature profile/ignition delay time and NOx concentrations, predicted with detailed and reduced mechanisms



Next steps

This example can be extended further

1. The reduced mechanism can be stored in CHEMKIN format and used directly in any engine CFD software, or used to calculate ignition delay time and laminar flame speed tables for engine combustion models, available in engine CFD codes
2. For stratified charge SI engines the range of stoichiometric conditions can be specified to make reduced mechanism working both lean and rich fuel-air mixtures
3. CO, PAH and unburned hydro-carbons (UHC) can be added as targets of mechanism reduction to extend the capabilities of the reduced mechanism to capture hydro-carbon emissions from SI engines
4. Prepare new project for reduction of detailed mechanism for diesel engine simulations

References

[1] E. Ranzi, A. Frassoldati, R. Grana, A. Cuoci, T. Faravelli, A.P. Kelley, C.K. Law, Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels, Progress in Energy and Combustion Science, 38 (4), pp. 468-501 (2012), DOI: 10.1016/j.pecs.2012.03.004